unknown substance, to determine in a short time the partial structures contained in the unknown substance based on the spectral data of the unknown substance, thereby making it possible for a spectroscopist or general chemist to easily and quickly determine the chemical structure. Further, the present invention does not require advanced skill and experience in spectroscopic techniques and eliminates the errors arising from the preconceptions and omissions to which human thought processes are so susceptible, thereby enabling the accurate determination of chemical structures.

What is claimed is:

1. An apparatus for determining the chemical structure of an unknown substance, comprising: a means for detecting spectral data of the unknown substance; a memory means for memorizing at least the chemical shift values corresponding to partial structures of known substances; a means for finding a point-assessment expressing the degree of possibility of partial structures being contained in the unknown substance based on the spectral data of the unknown substance and the data stored in said memory means; comparison means for judging whether said point-assessment is a predetermined threshold value or more; and an output means for displaying the partial structures with a large possibility of being contained in the unknown substance based on the output of said comparison means.

2. An apparatus according to claim **1**, wherein said partial structures include carbon atoms and non-carbon atoms bonded to said carbon atoms.

3. An apparatus according to claim **1**, wherein said means for detecting spectral data of an unknown substance is a C-13 NMR apparatus.

4. An apparatus according to claim **1**, wherein said point-assessment is obtained by sequentially deriving data for each partial structure, by calculating membership function $\phi(t)_i$ for every spectral data of each partial structure emcompassed in the unknown substance according to the following formulas:

$$t_i = \frac{|P_0 - P_k|}{\sigma}$$

$$\phi(t)_i = \exp\left(-\tfrac{1}{2}t_i^2\right)$$

wherein P_0 is the central freuency, P_k is the frequency of each spectral data, and σ is the standard deviation, and by calculating the weighted average ϕ_T of the membership functions of said spectral data of said partial structure according to the following formula:

$$\phi_T = \frac{W_1\phi(t)_1 + W_2\phi(t)_2 + \ldots}{W_1 + W_2 + \ldots}$$

wherein W_1, W_2, ... are weights of said spectral data, said weighted average ϕ_T being used as said point-assessment.

5. An apparatus according to claim **4**, wherein said membership function is calculated only for every input spectral data whose number of splitting patterns coincides with the number of splitting patterns of the spectral data of the partial structure.

6. An apparatus according to claim **1**, wherein said memory means stores a chemical shift table including at least the central position and the standard deviation of each spectral signal for every partial structure.

7. An apparatus according to claim **6**, wherein said chemical shift table further includes weight data for every spectral signal.

8. An apparatus according to claim **6**, wherein said chemical shift table further includes splitting pattern data for every spectral signal.

9. An apparatus according to claim **1**, wherein said memory means stores the chemical shift values corresponding to a plurality of aromatic ring partial structures of known substances.

10. An apparatus according to claim **9**, wherein said chemical shift values include data of highest and lowest positions of the shift range of the spectral signal of every partial structure.

11. An apparatus according to claim **9**, wherein said point-assessment is obtained by sequentially deriving data for each aromatic ring partial structure, by calculating membership function $\phi(t)_i$ for every spectral data of each aromatic ring partial structure emcompassed in the unknown substance according to the following formulas:

$$t_i = \frac{|P_0 - P_k|}{\sigma}$$

$$\phi(t)_i = \exp\left(-\tfrac{1}{2}t_i^2\right)$$

wherein P_0 is the central frequency, P_k is the frequency of each spectral data, and σ is the standard deviation, by combining aromatic ring partial structures each having membership function equal to or larger than a predetermined threshold value so as to form a ring structure, and by calculating the weighted average ϕ_T of the membership functions of said spectral data of said partial structures according to the following formula:

$$\phi_T = \frac{W_1\phi(t)_1 + W_2\phi(t)_2 + \ldots}{W_1 + W_2 + \ldots}$$

wherein W_1, W_2, ... are weights of said spectral data, said weighted average ϕ_T being used as said point-assessment.

12. An apparatus according to claim **11**, wherein said membership function is calculated only for every input spectral data whose number of splitting patterns coincides with the number of splitting patterns of the spectral data of the aromatic ring partial structure.

13. A method for determining the chemical structure if an unknown substance comprising detecting spectral data of the unknown substance, finding a point-assessment expressing the degree of possibility of partial structure being contained in the unknown substance based on said spectral data and prememorized chemical shift values corresponding to the partial structures of known substances, judging whether said point-assessment is a predetermined threshold value or more, thereby producing judgement results, and finding and displaying the partial structures with a large possibility of being contained in the unknown substance based on the output of said judgement results.

14. A method according to claim **13**, wherein said partial structures include carbon atoms and non-carbon atoms bonded to said carbon atoms.

15. A method according to claim **13**, wherein said spectral data of an unknown substance is detected by a C-13 NMR apparatus.